Solving L_0-Problems via Mixed-Integer Optimization

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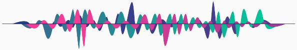
LS2N seminar
7th of March, 2024
Nantes, France

Sparse Optimization

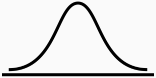
Two goals, one problem

Minimize a function $\xleftrightarrow{\textbf{Sparse optimization}}$ **Sparse solution**



Signal processing

Machine learning



High-dim. statistics

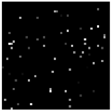
And many others

Signal processing

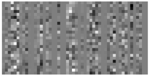
Compressive sensing

Linear measurement through $A \in \mathbb{R}^{m \times n}$

Sparse signal
$x \in \mathbb{R}^n$



Observation
$y \in \mathbb{R}^m$



Recover x from (A, y)

Find x **such that** $y \simeq Ax$

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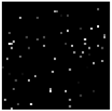

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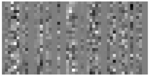

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$m \ll n$: no unique solution

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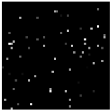

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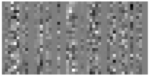

Recover x from (A, y)

Find x **sparse such that** $y \simeq Ax$

$m \ll n$: no unique solution

High-dimensional statistics

Sparse GLM

Features $\mathrm{A} \in \mathrm{R}^{m \times n}$

Targets $\mathrm{y} \in \mathrm{R}^{m}$

↓

$\max_{\mathrm{x}} \; \mathcal{L}(\mathrm{Ax}, \mathrm{y})$

No unique solution when $m \ll n$

↓

$\max_{\mathrm{x}} \; \mathcal{L}(\mathrm{Ax}, \mathrm{y})$ with x sparse

High-dimensional statistics

Sparse GLM	**Sparse PCA**
Features $A \in \mathbb{R}^{m \times n}$	Features $A \in \mathbb{R}^{m \times n}$
Targets $y \in \mathbb{R}^{m}$	Covariance $\Sigma = A^{\mathrm{T}}A$
↓	↓
$\max_{x} \; \mathcal{L}(Ax, y)$	$\max_{\lVert x \rVert_2 = 1} \; x^{\mathrm{T}}\Sigma x$
No unique solution when $m \ll n$	Not relevant when $m \ll n$
↓	↓
$\max_{x} \; \mathcal{L}(Ax, y)$ with x sparse	$\max_{\lVert x \rVert_2 = 1} \; x^{\mathrm{T}}\Sigma x$ with x sparse

Machine learning

Heart disease dataset (LIBSVM)

Age	Sex	Cholesterol	Blood pressure	...	**Disease**
31	M	50.3 mg/dl	95 mm/hg	...	**No**
35	F	54.9 mg/dl	98 mm/hg	...	**Yes**
42	F	49.8 mg/dl	92 mm/hg	...	**Yes**
37	M	59.1 mg/dl	89 mm/hg	...	**No**
...	...	...	...	...	...

Machine learning

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Data $\longrightarrow$ **Logistic regression** $\longrightarrow$ **Estimator** x

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Data $\longrightarrow$ **Logistic regression** $\longrightarrow$ **Estimator** x

Involves all the features

Explainability and robustness issues

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Data $\longrightarrow$ **Logistic regression** $\longrightarrow$ **Estimator** x

Force the use of only few features via sparsity in x

Involves all the features
Explainability and robustness issues

Objective, constraint or both ?

Minimize a function $\longleftrightarrow$ **Sparse optimization** $\longleftrightarrow$ **Sparse solution**

Loss function $F(x)$

Counting function $\|x\|_0$

Objective, constraint or both ?

Minimize a function $\longleftrightarrow$ **Sparse optimization** $\longleftrightarrow$ **Sparse solution**

Loss function $F(\mathrm{x})$

Counting function $\|\mathrm{x}\|_0$

Constrainted version

$$\begin{cases} \min_{\mathrm{x}} & F(\mathrm{x}) \\ \text{s.t.} & \|\mathrm{x}\|_0 \leq s \end{cases}$$

Minimized version

$$\begin{cases} \min_{\mathrm{x}} & \|\mathrm{x}\|_0 \\ \text{s.t.} & F(\mathrm{x}) \leq \epsilon \end{cases}$$

Penalized version

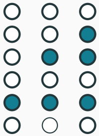
$$\min_{\mathrm{x}} F(\mathrm{x}) + \lambda\|\mathrm{x}\|_0$$

A bit of history

1990

Sparse
heuristics

MP, OMP,
IHT and co.



A bit of history

1990 | **2000**

Sparse heuristics

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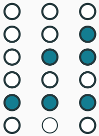

Formulation with ℓ_0-norm

RIP, NSP,
EkR and co.

OMP
|||
ℓ_0-prob.

A bit of history

1990

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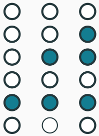


2000

Formulation with ℓ_0-norm

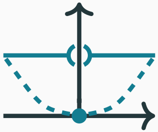
RIP, NSP, EkR and co.

OMP
|||
ℓ_0-prob.

2005

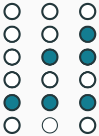
Convex approx. of ℓ_0-norm

Lasso, Elastic-Net and co.

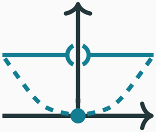


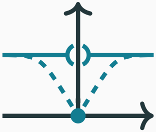
A bit of history

1990	2000	2005	2013
Sparse heuristics	Formulation with ℓ_0-norm	Convex approx. of ℓ_0-norm	Concave approx. of ℓ_0-norm
MP, OMP, IHT and co.	RIP, NSP, EkR and co.	Lasso, Elastic-Net and co.	SCAD, MCP CEL0 and co.



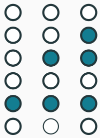
OMP $\equiv$ ℓ_0-prob.





A bit of history

1990	2000	2005	2013	2016
Sparse heuristics	Formulation with ℓ_0-norm	Convex approx. of ℓ_0-norm	Concave approx. of ℓ_0-norm	Exact methods for ℓ_0-norm
MP, OMP, IHT and co.	RIP, NSP, EkR and co.	Lasso, Elastic-Net and co.	SCAD, MCP CEL0 and co.	MIP, BnB CP and co.



OMP
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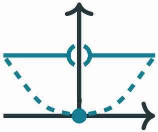
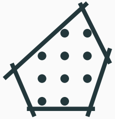
ℓ_0-prob.





Mixed-Integer Optimization

Handeling the L0-norm with MIO tools

Problem

$\min_x F(x) + \lambda \|x\|_0$

$\downarrow$ Solver

Solution

Handeling the L0-norm with MIO tools

Problem

$\min_x F(x) + \lambda \|x\|_0$

Solver

Solution

Non-linear, non-convex,
non-smooth, NP-hard, ...

😵

Handeling the L0-norm with MIO tools

Problem

$\min_x F(x) + \lambda \|x\|_0$

Solver

Solution

Non-linear, non-convex,
non-smooth, NP-hard, ...

The ℓ_0-norm counts the number of non-zeros in vector x

It sums the entries of the binary vector z satisfying some logical relation with x

We have tools to deal with such binary vectors in MIO !

Fitting the MIO formalism

Linearizing the ℓ_0-norm

Real vector $x \in \mathbb{R}^n$ and binary vector $z \in \mathbb{B}^n$:

$$\|x\|_0 = 1^{\mathrm{T}} z \quad \text{if} \quad x \odot (1 - z) = 0$$

Fitting the MIO formalism

Linearizing the ℓ_0-norm

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$$\boxed{\min_x F(x) + \lambda \|x\|_0}$$

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$$\boxed{\min_x F(x) + \lambda \|x\|_0}$$

$$\downarrow$$

$$\boxed{\min_{x,z} F(x) + \lambda 1^{\mathrm{T}} z + H(x, z)}$$

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$$\boxed{\min_{x,z} F(x) + \lambda 1^{\mathrm{T}} z + H(x, z)}$$

$$\downarrow$$

$$\boxed{\begin{aligned} \min_{x,z} \quad & F(x) + \lambda 1^{\mathrm{T}} z \\ \text{s.t.} \quad & -Mz \le x \le Mz \end{aligned}}$$

Fitting the MIO formalism

Linearizing the ℓ_0-norm

Real vector $x \in \mathbb{R}^n$ and binary vector $z \in \mathbb{B}^n$:

$$\|x\|_0 = \mathbf{1}^{\mathrm{T}} z \quad \text{if} \quad x \odot (\mathbf{1} - z) = 0$$

$$\boxed{\min_x F(x) + \lambda \|x\|_0}$$

$$\downarrow$$

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$$\downarrow$$

$$\boxed{\begin{array}{rl} \min_{x,z} & F(x) + \lambda \mathbf{1}^{\mathrm{T}} z \\ \text{s.t.} & -Mz \leq x \leq Mz \end{array}}$$

Generic MIO solvers (Cplex, Gurobi, ...)
✗ Slow ✓ Generic w.r.t F/H

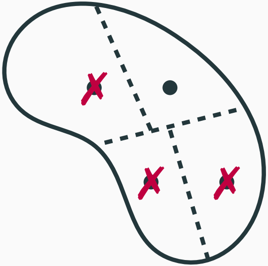
Specialized solvers (BnB, CP, ...)
✓ Fast ✗ Resticted to some F/H

Specialized Solution Methods

Branch-and-Bound algorithms

Branch-and-Bound

"Enumerate all candidate solutions and discard sub-optimal ones."



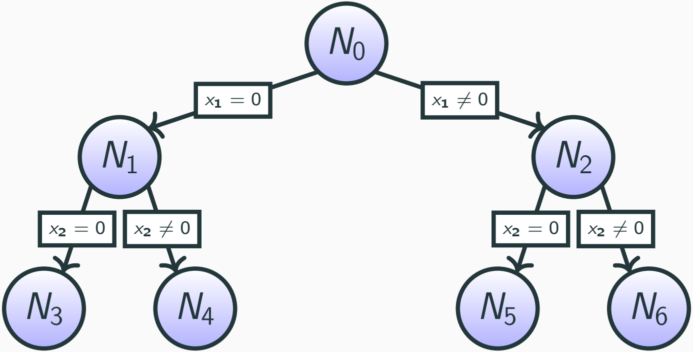
Main principles

Branching: Divide the search space

Bounding: Test whether a region can contain optimal solutions

Pruning: Discard regions without optimal solutions

Tree exploration



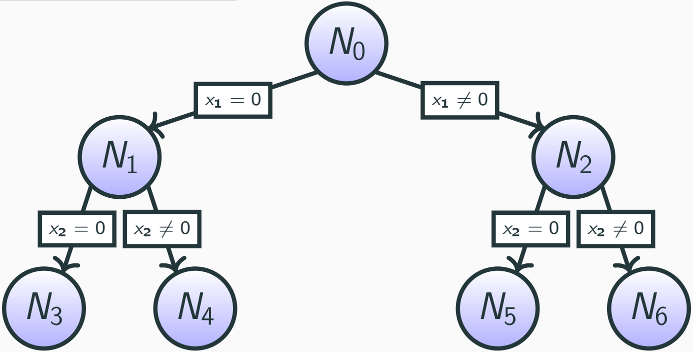
Tree exploration

Observation

If support of x is fixed, then

$$\min_{x} F(x) + \lambda\|x\|_0 + H(x)$$

is easy to solve.



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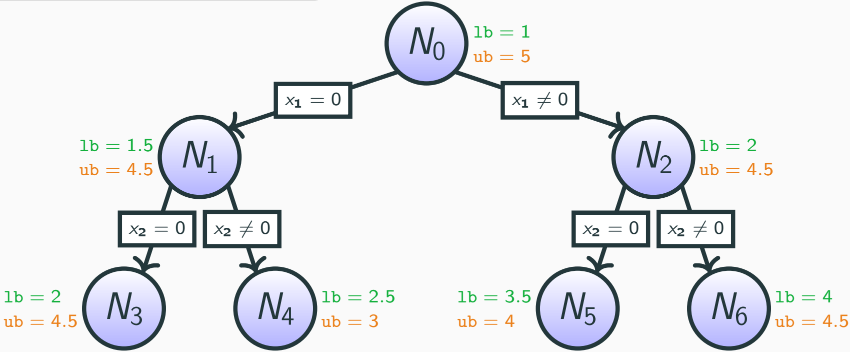

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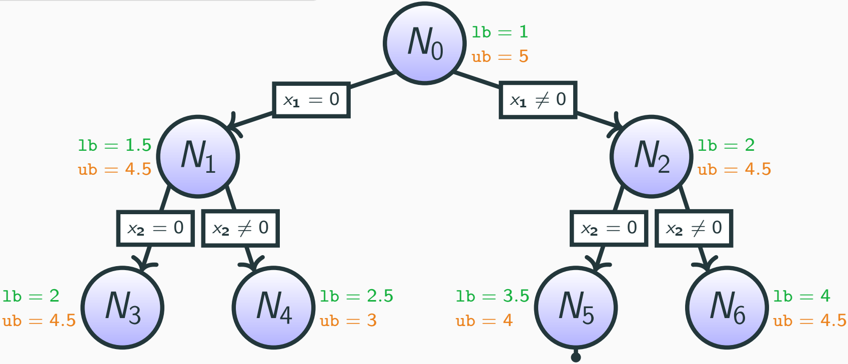

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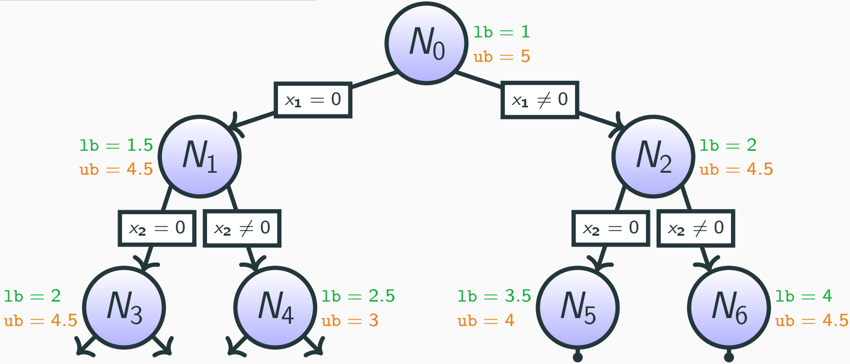

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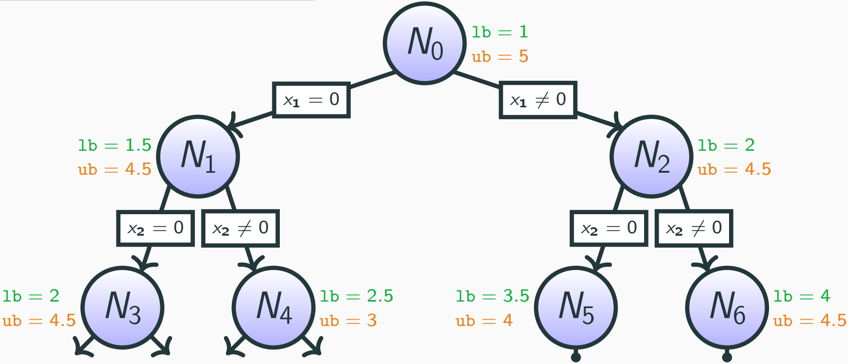

All nodes explored or pruned $\longrightarrow$ Problem solved

Node processing

$(\mathcal{S}_0, \mathcal{S}_1)$

Node problem

The problem at node $\nu = (\mathcal{S}_0, \mathcal{S}_1)$ where $\mathcal{S}_0$ and $\mathcal{S}_1$ are the indices of x fixed to zero and non-zero reads

$$p^{\nu} = \begin{cases} \min_{\mathbf{x}} & F(\mathbf{x}) + \lambda\|\mathbf{x}\|_0 + H(\mathbf{x}) \\ \text{s.t.} & \mathbf{x}_{\mathcal{S}_0} = 0,\ \mathbf{x}_{\mathcal{S}_1} \neq 0 \end{cases}$$

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Task: Find lower and upper bounds on p^ν that are **tight** and **tractable to compute**

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Task: Find lower and upper bounds on p^ν that are **tight** and **tractable to compute**

Upper bounding

- We just need a feasible solution
- Fix entries of x that are still free to zero
- Optimize the resulting problem

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$(\mathcal{S}_0, \mathcal{S}_1)$

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Task: Find lower and upper bounds on p^ν that are **tight** and **tractable to compute**

Upper bounding

- We just need a feasible solution
- Fix entries of x that are still free to zero
- Optimize the resulting problem

Easy to solve

Upper-bounding problem

$$\min_{\mathrm{x}}\ F(\mathrm{x}_{\mathcal{S}_1}) + \lambda|\mathcal{S}_1| + H(\mathrm{x}_{\mathcal{S}_1})$$

Lower bounding

Idea: Convexify a part of the objective function

Node problem

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$\min_{\mathrm{x}} F(\mathrm{x}) + G(\mathrm{x})$

Lower bounding

Idea: Convexify a part of the objective function

Node problem

$$p^\nu = \begin{cases} \min_x & F(x) + \lambda\|x\|_0 + H(x) \\ \text{s.t.} & x_{\mathcal{S}_0} = 0,\ x_{\mathcal{S}_1} \neq 0 \end{cases}$$

$\min_x F(x) + G(x)$

$\boxed{\text{Bi-conjugacy } G^{\star\star}(x) \leq G(x)}$

Lower-bounding problem

$$\min_x F(x) + G^{\star\star}(x)$$

Lower bounding

Idea: Convexify a part of the objective function

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$\min_x F(x) + G(x)$

$\boxed{\text{Bi-conjugacy } G^{\star\star}(x) \leq G(x)}$

Lower-bounding problem

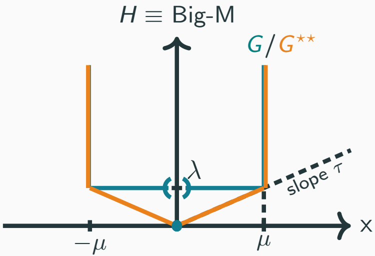
$$\min_x F(x) + G^{\star\star}(x)$$

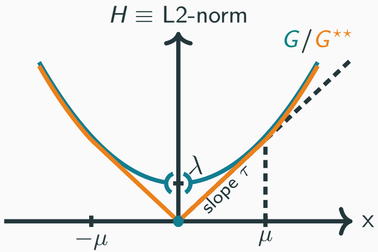
Closed-form expression

🥳

H proper, closed, coercive continuous at its minimum

Graphical intuition





Bi-conjugate closed-form

$$G^{\star\star}(x) = \begin{cases} \tau|x| & \text{if } |x| \leq \mu \\ G(x) & \text{otherwise} \end{cases}$$

Let's sum up !

ℓ_0-penalized problem

$$\min_x \; F(x) + \lambda \|x\|_0 + H(x)$$

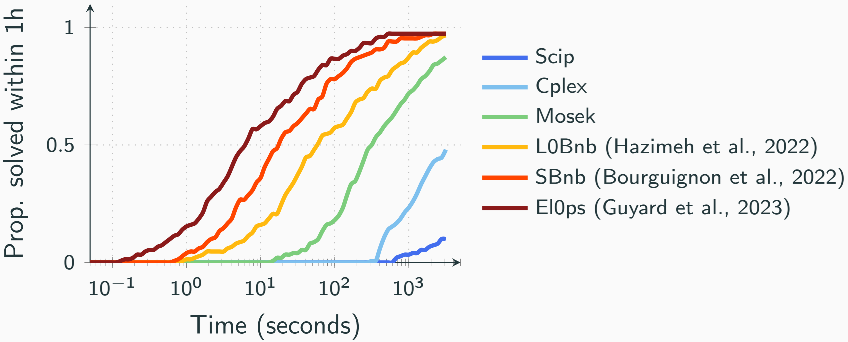
- MIP formalism
  - Linearize the ℓ_0-norm with a binary variable
  - Big-M strategy
- Generic solvers
  - Easy solution to implement
  - Unable to exploit sparsity
  - Numerically inefficient
- Specialized Branch-and-Bound
  - Tree exploration
  - Branch by fixing support of x
  - Compute upper and lower bounds at each node
  - Leverage bi-conjugacy to compute lower bounds

Overview of Numerical Performances

Overview of numerical performances

$$\min_x \; F(x) + \lambda\|x\|_0 + H(x)$$

Dataset : Sparse regression
F(·) : Least-squares loss
H(·) : Big-M constraints
λ : Set statistically



Overview of numerical performances

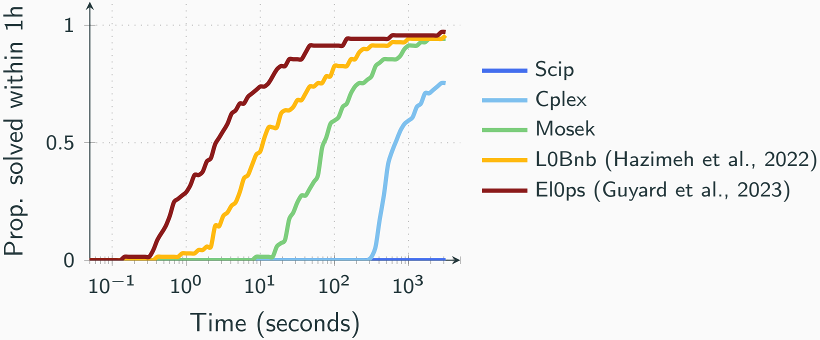
$$\min_x \; F(x) + \lambda\|x\|_0 + H(x)$$

Dataset : Sparse regression

F(·) : Least-squares loss

H(·) : L2-norm

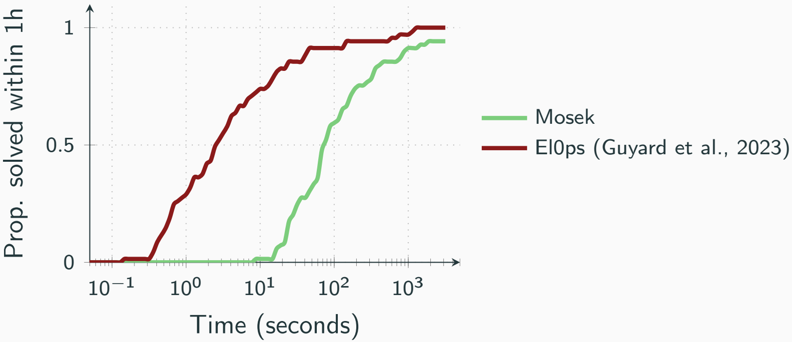
λ : Set statistically



Overview of numerical performances

$$\min_x \; F(x) + \lambda\|x\|_0 + H(x)$$

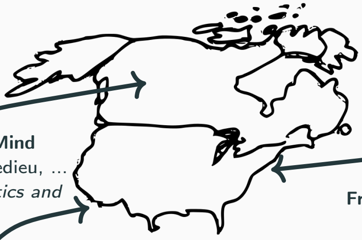
Dataset : Sparse classification
F(·) : Logistic loss
H(·) : L1-norm
$\boldsymbol{\lambda}$: Set statistically



Ongoing Research Directions

Contributors and research works

Non-exhaustive list



MIT
D. Bertsimas, R. Mazmuder, ...
MIO tools for ℓ_0-problems

Lund University
M. Carlsson, C. Olsson...
Quadratic envelope

Google Deep Mind
H. Hazimeh, A. Dedieu, ...
MIO-based heuristics and softwares

Frankfurt / Wurzburg Universities
C. Kanzow, A. Tillmann, ...
Optimality conditions

Berkley
A. Atamtürk, A. Gomès, ...
Convex-based acceleration

London Business School
J. Pauphilet, R. Cory-Wright, ...
Healthcare applications

Ponts ParisTech
M. De Lara, P. Chancelier, A. Parmentier, ...
Non-convex analysis for ℓ_0-norm, ML appli.

Centrale Nantes / ENSTA Bretagne
S. Bourguignon, J. Ninin, ...
Branch-and-Bound for ℓ_0-problems

Inria / CentraleSupélec
C. Herzet, C. Elvira, A. Arslan, ...
Generalization, acceleration

IRIT / I3S
E. Soubies, L. Blanc-Féraud, ...
Strong relax. of ℓ_0-norm

Take-home message

- In some cases, solving ℓ_0-norm problems exactly worths-it
- There exists Mixed-Integer Optimization tools to do so
- Structure exploitation is the key to achieve competitive performances
- Active research area

  $\rightarrow$ Theoretical results

  $\rightarrow$ Efficiency, flexibility and accessibility of solution methods

  $\rightarrow$ Software development

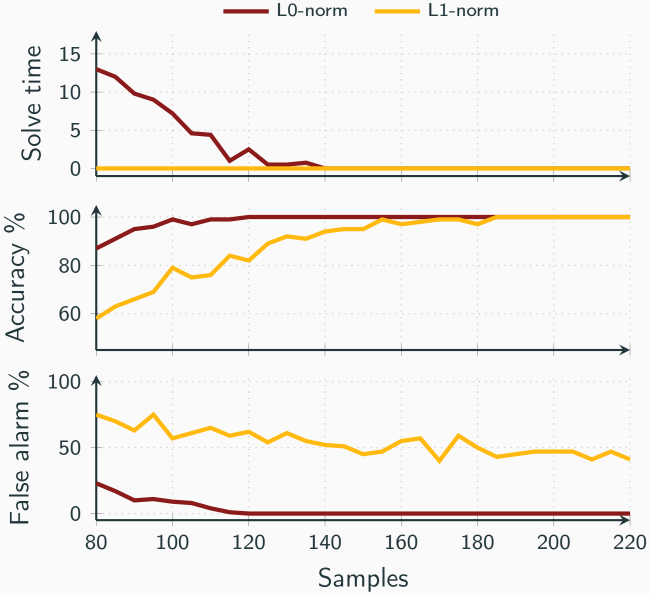
  $\rightarrow$ Diffusion to other communities

Question time

🤓

Supplementary Slides

Why solving L0 problems ?



Sparse regression

$y = Ax^{\dagger} + \epsilon$

2.000 features

10 non-zeros in $x^{\dagger}$

20dB noise

D. Bertsimas and B. Van Parys, Sparse High-Dimensional Regression: Exact Scalable Algorithms and Phase Transitions